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NUMERICAL METHODS FOR TRANSIENT
SEMICONDUCTOR DEVICE MODELLING

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ABSTRACT

A mixed system of parabolic and elliptic partial differential equations
is used to describe the carrier transport and potential distribution in semi-
conductor devices such as MOSFET's, diodes, etc. A singular perturbation
analysis of the corresponding initial boundary value problem is carried out.
Asymptotic expansions of the solution in powers of the minimal Debeye length
are given. Based on this analysis a finite difference method for the
numerical solution of these problems is developed. Here problems arise due to
different time scales which are intrinsically present in the analytical
problem. These different time scales do not occur in the physical solutions
because of special (equilibrium-) initial conditions. Nevertheless they cause
severe stability problems for finite difference methods. An unconditionally
stable scheme is developed which minimizes computational effort. Numerical
experiments on a test problem in one space dimension are presented.

AMS (MOS) Subject Classifications: 35G25, 35M05, 65M15

Key Words: Semiconductors, Singular Perturbations, Finite Difference Methods

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SIGNIFICANCE AND EXPLANATION

In this paper we are concerned with a one dimensional transient model for a simple p – n junction (i.e. a diode). The model consists of an initial boundary value problem for a singularly perturbed nonlinear system of elliptic and parabolic P.D.E.'s in one space and one time dimension. One of the main purposes of this model is to give information about the "rise-time" of the p – n junction (the time required to reach a steady state). We carry out our asymptotic analysis of the problem for large doping concentrations. (This is the case for modern devices.) We derive asymptotic expansions of the solution in powers of a singular perturbation parameter which is proportional to the minimal Debeye-length of the device. It turns out that the solutions vary on a time scale which is proportional to the average lifetime of electrons and holes. Therefore the risetimes will be of the same order of magnitude as this lifetime. In addition to this timescale there is a second "first" timescale intrinsically present in the problem. This first timescale – although never observed physically because of special (equilibrium-) initial conditions – causes severe stability problems in the numerical solution of the problem. Based on our asymptotic analysis we derive an unconditionally stable finite difference method for the solution of the p – n junction equations.
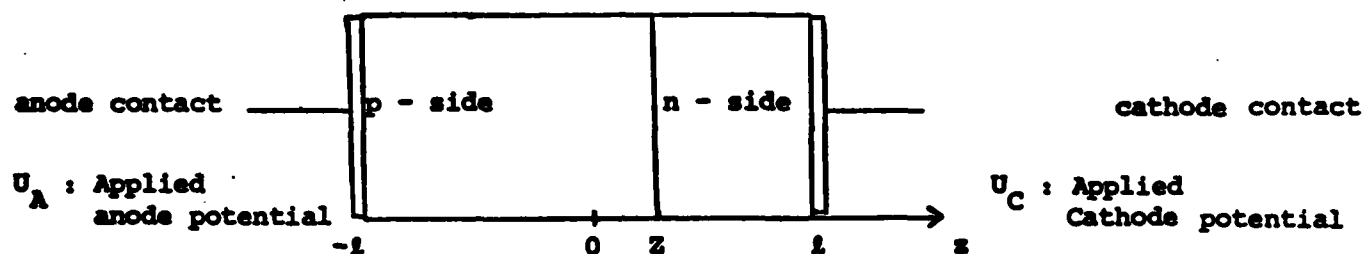
NUMERICAL METHODS FOR
TRANSIENT SEMICONDUCTOR DEVICE MODELLING

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1. Introduction

In this paper we present an asymptotic analysis of a singularly perturbed mixed system of parabolic and elliptic differential equations modelling a p - n junction. The physical situation is as follows: A semiconductor (for instance silicone) is doped with acceptor atoms in the left hand side and donor atoms in the right hand side and a bias $U = U_A - U_C$ is applied to the contacts.

anode contact _____ | p - side | n - side | _____ cathode contact

U_A : Applied anode potential

U_C : Applied Cathode potential

-ℓ   0   z   ℓ   z

The device is assumed to have a characteristic length 2ℓ ($\sim 0.5*10^{-3}$cm) and the junction is at $x = 0$. The device is forward biased for $U > 0$ and reverse biased for $U < 0$. The physics of a p - n junction is explained in Sze [1969], Ashcroft et al [1976] and R. A. Smith [1978]. The equations describing the electrostatic potential and the carrier and current densities were first given by Van Roosebroeck in [1950]. In the case of one space dimension they consist of

(1.1) $\psi_{xx} = \frac{q}{\varepsilon} (n - p - C)$ (Poisson's equation)

(1.2) $J_n = q(D_n n_x - \mu_n n \psi_x)$ electron current relation

(1.3) $J_p = -q(D_p p_x + \mu_p p \psi_x)$ hole current relation

(1.4) $\qquad n_t = \frac{1}{q} J_{n_x} + R \qquad$ continuity equations

(1.5) $\qquad p_t = -\frac{1}{q} J_{p_x} + R \qquad$ for electrons and holes.

The system (1.1) to (1.5) is subject to the boundary conditions

(1.6) $\qquad \psi(-\ell,t) = U_T \ln\left(\frac{n_i}{p(-\ell,t)}\right) + U_A(t)$

(1.7) $\qquad \psi(\ell,t) = U_T \ln\left(\frac{n_i}{n(\ell,t)}\right) + U_C(t)$

(1.8) $\qquad n(\pm\ell,t)\, p(\pm\ell,t) = n_i^2$

(1.9) $\qquad n(\pm\ell,t) - p(\pm\ell,t) - C(\pm\ell) = 0$

and the initial conditions

(1.10) $\qquad\qquad \psi(x,0) = \psi_I(x)$

(1.11) $\qquad\qquad n(x,0) = n_I(x)$

(1.12) $\qquad\qquad p(x,0) = p_I(x)$

The dependent variables (with units) are

Table 1

ψ electric potential (V)

ψ_x electric field (Vcm^{-1})

n electron density (cm^{-2})

p hole density (cm^{-3})

J_n electron current density (Acm^{-2})

J_p hole current density (Acm^{-2}) .

The parameters q, ε, μ_n, μ_p, D_n, D_p, n_i, U_T in (1.1) – (1.5) have the following meaning and approximate values at $T \approx 300K$ (room temperature)

Table 2

q	elementary charge	10^{-19}As
ϵ	permittivity constant	10^{-12}As/Vcm^3
μ_n	electron mobility	10^3cm^2/(Vs)
μ_p	hole mobility	10^3cm^2/(Vs)
n_i	intrinsic density	10^{10}cm^{-3}
$U_T = \dfrac{D_n}{\mu_n} = \dfrac{D_p}{\mu_p}$	thermal voltage	0.025V

C is a given function of x and models the doping profile, i.e.

(1.13) $$C(x) = N_D^+(x) - N_A^-(x) \quad (cm^{-3})$$

where N_D^+ and N_A^- are the densities of electrically active donor and acceptor atoms in the doped semiconductor. C(x) is negative for x < 0 (on the p-side) and positive for x > 0 (on the n-side). We further assume that C is an odd function i.e.

(1.14) $$C(x) = -(C-x) \quad \text{holds.}$$

(Although this does not appear to be any special case from the physical point of view it will simplify the analysis considerably.) We assume that C(x) has a jump-discontinuity at x = ∅. R in (1.4), (1.5) denotes the generation-recombination term and describes the rate at which electron hole carrier pairs are generated or recombine (vanish). For our purpose it suffices to consider the Shockley-Read-Hall recombination term

(1.15) $$R = R_{SRH}(n,p) = \frac{np - n_i^2}{\tau_p(n+n_i) = \tau_n(p+n_i)} \quad (cm^{-3}s^{-1}) \quad .$$

τ_n and τ_p denote the average lifetimes of electron and holes. For simplicity we set $\tau_n = \tau_p = \tau = 10^{-6}$(s). Other mote realistic recombination rates are given in Langer et al [1981] and Schütz et al [1981]. In general it

can be said that the choice of the recombination rate is not very important for the behavior of solutions of the time dependent problem (whereas it is in the steady state case - see Markowich and Ringhofer [1983], Markowich et al [1983a], Mock [1983] and Schütz et al [1982]).

A more restrictive assumption is $\mu_n = \mu_p = const$. In general μ_n and μ_p can be modelled as functions of the electric field ψ_x. This might influence the behavior of the solutions considerably (see c.f. Mock [1983]).

For the rest of this paper we assume that the initial conditions (1.10) - (1.12) are compatible with the boundary conditions and the differential equation. So we assume that

$$(1.16) \qquad \psi_{I_{xx}} = \frac{q}{\varepsilon}(n_I - p_I - C)$$

$$(1.17) \qquad n_I(\pm\ell) \cdot p_I(\pm\ell) = n_i^2$$

$$(1.18) \qquad n_I(\pm\ell) - p_I(\pm\ell) - C(\pm\ell) = 0$$

$$(1.19) \qquad \psi_I(-\ell) = U_T \ln\left(\frac{n_i}{p_I(-\ell)}\right) + U_A(0)$$

$$(1.20) \qquad \psi_I(\ell) = U_T \ln\left(\frac{n_i}{n_I(\ell)}\right) + U_C(0)$$

holds.

After an appropriate scaling we carry out an asymptotic analysis of the problem (1.1) - (1.12) where the (dimensionless) quantity

$$(1.21) \qquad \lambda = \left(\frac{\varepsilon U_T}{q \max_{x \in [-\ell,\ell]} |C(x)| \ell^2}\right)^{1/2}$$

acts as a perturbation parameter.

We investigate the behavior of the solutions as $\lambda \to 0$ which corresponds to very high doping (which is the case for modern devices). It turns out that there are two different timescales intrinsically present in the equations

(1.1) – (1.5). However if we choose the initial conditions ψ_I, n_I and p_I in (1.10) – (1.12) to be the solutions of the steady state problem

(1.22)
$$\psi_{xx} = \frac{q}{\epsilon}(n - p - C)$$

(1.23)
$$J_n = q(D_n n_x - \mu_n n \psi_x)$$

(1.24)
$$J_p = -q(D_p p_x + \mu_p p \psi_x)$$

(1.25)
$$J_{n_x} = R \quad , \quad J_{p_x} = -R$$

the solutions will vary only on the "slow" time scale (which is of the same order of magnitude as τ the average lifetime of electrons and holes). Although the other ("fast") time scale is not present in this case, it causes severe stability problems for numerical methods to solve (1.1) – (1.12). We derive a finite difference method for problem (1.1) – (1.12) which is unconditionally stable and of second order in time. At each time step the solution of two coupled nonlinear differential equations is required. The generalization of this method to nonsymmetric $p - n$ junctions (i.e. $C(x)$ not odd) and to two or three space dimensions is straightforward.

This paper is organized as follows. In Chapter 2 we scale problem (1.1) – (1.12) and reformulate it as a singular perturbation problem. In Chapter 3 we review the asymptotic analysis for the steady state problem (1.22) – (1.25) given in Markowich and Ringhofer [1982] and Markowich et al [1982]. In Chapter 4 we derive the asymptotic expansion of the solution of (1.1) – (1.12). In Chapter 5 we construct the finite difference method. In Chapter 6 we present some numerical results on a test problem.

2. Reformulation as a singular perturbation problem

In this chapter we scale the system (1.1) - (1.5) appropriately and transform it into a singular perturbation problem. Essentially we use the scaling given in Markowich and Ringhofer [1982] and Markowich et al [1983a]. We scale the independent variables x and t by the characteristic length of the device and by the average lifetime of electrons and holes.

(2.1)
$$x_s = \frac{x}{\ell} \quad , \quad t_s = \frac{t}{\tau} \quad .$$

For the dependent variables ψ, n, p, J_n and J_p we employ the following scaling:

(2.2)
$$\psi_s = \frac{\psi}{U_T} \quad , \quad n_s = \frac{n}{\bar{C}} \quad , \quad p_s = \frac{p}{\bar{C}}$$

(2.3)
$$J_{n_s} = \frac{\ell}{\bar{C}qD_n} J_n \quad , \quad J_{p_s} = \frac{\ell}{\bar{C}qD_p} J_p$$

(2.4)
$$\bar{C} := \max_{x \in [-\ell,\ell]} |C(x)| \quad .$$

In this scaling equations (1.1) - (1.5) assume the form

(2.5)
$$\lambda^2 \frac{\partial^2}{\partial x_s^2} \psi = n_s - p_s - C_s$$

(2.6)
$$\frac{\partial}{\partial t_s} n_s = \frac{\tau D_n}{\ell^2} \frac{\partial}{\partial x_s} J_{n_s} + R_s$$

(2.7)
$$\frac{\partial}{\partial t_s} p_s = - \frac{\tau D_p}{\ell^2} \frac{\partial}{\partial x_s} J_{p_s} + R_s$$

(2.8)
$$J_{n_s} = \frac{\partial}{\partial x_s} n_s - n_s \frac{\partial}{\partial x_s} \psi_s$$

(2.9)
$$J_{p_s} = - \frac{\partial}{\partial x_s} p_s - p_s \frac{\partial}{\partial x_s} \psi_s$$

(2.10)
$$\lambda := \left(\frac{\varepsilon U_T}{\ell^2 q \bar{C}}\right)^{1/2} \quad , \quad C_s(x_s) = \frac{C(x)}{\bar{C}}$$

(2.11)
$$R_s = (n_s p_s - \alpha^2)(n_s + p_s + 2\alpha)^{-1} , \quad \alpha := \frac{n_i}{\bar{C}} \quad .$$

The boundary conditions (1.6) - (1.9) transforms to

$$(2.12) \qquad n_s = \frac{1}{2} (C_s + \sqrt{C_s^2 + 4\alpha^2})$$

$$\text{at} \quad x_s = \pm 1$$

$$(2.13) \qquad p_s = \frac{1}{2} (-C_s + \sqrt{C_s^2 + 4\alpha^2})$$

$$(2.14) \qquad \psi_s(-1, t_s) = \frac{U_A(t_s)}{U_T} + \ln\left(\frac{n_s(-1)}{\alpha}\right)$$

$$(2.15) \qquad \psi_s(1, t_s) = \frac{U_C(t_s)}{U_T} + \ln\left(\frac{n_s(1)}{\alpha}\right) \quad .$$

The initial conditions transform to

$$(2.16) \qquad \psi_s(x_s, 0) = \psi_s^I(x_s) = \frac{1}{U_T} \psi^I(x)$$

$$(2.17) \qquad n_s(x_s, 0) = n_s^I(x_s) = \frac{1}{C} n^I(x)$$

$$(2.18) \qquad p_s(x_s, 0) = p_s^I(x_s) = \frac{1}{C} p^I(x) \quad .$$

The quantities in (2.5) - (2.18) are now dimensionless. Using the numerical values given in Table 2 for the physical parameters gives (after omitting the subscript s)

$$(2.19) \qquad \lambda^2 \psi_{xx} = n - p - C$$

$$(2.20) \qquad n_t = J_{n_x} + R \quad , \quad p_t = -J_{p_x} + R$$

$$(2.21) \qquad J_n = n_x - n\psi_x \quad , \quad J_p = -p_x - p\psi_x$$

together with the boundary conditions

$$(2.22) \quad \psi(-1, t) = \psi_{-1}(t) \quad , \quad \psi(1, t) = \psi_1(t)$$

$$(2.23) \quad n = \frac{1}{2} (C + \sqrt{C^2 + 4\alpha^2}) \quad , \quad p = \frac{1}{2} (-C + \sqrt{C^2 + 4\alpha^2}) \quad , \quad x = \pm 1$$

where ψ_{-1} and ψ_1 are given by

$$\psi_{-1}(t) = \frac{1}{U_T} U_A(t) + \ell n\left(\frac{C(-1) + \overline{\sqrt{C(-1)^2 + \psi\alpha^2}}}{2\alpha}\right)$$

$$\psi_1(t) = \frac{1}{U_T} U_C(t) + \ell n\left(\frac{C(1) + \overline{\sqrt{C(1)^2 + \psi\alpha^2}}}{2\alpha}\right)$$

$$\alpha := n_i/\overline{C}$$

and the initial conditions

(2.24) $\qquad \psi(x,0) = \psi^I(x), \; n(x,0) = n^I(x), \; p(x,0) = p^I(x) \quad .$

(2.19) - (2.24) represents a singularly perturbed system consisting of an

elliptic equation (2.19) and two parabolic conservation laws (2.20) -

(2.21). The compatibility conditions (1.16) - (1.20) now read

(2.25) $\quad \psi^I(-1) = \psi_{-1}(0), \; \psi^I(1) = \psi_1(0)$

(2.26) $\quad n^I = \frac{1}{2} (C + \overline{\sqrt{C^2 + 4\alpha^2}}), \; p^I = \frac{1}{2} (-C + \overline{\sqrt{C^2 + 4\alpha^2}}), \; x = \pm 1$

(2.27) $\quad \lambda^2 \psi^I_{xx} = n^I - p^I - C \quad .$

In the following chapters we will carry out our asymptotic analysis for (2.19)

- (2.24) for $\lambda \to 0$ which corresponds to very high doping $(\overline{C} \to \infty)$. This

usually is the case for modern devices. For the set of parameters given in

Table 2 of Chapter 1 and a maximal doping $\overline{C} \approx 10^{17} cm^{-3}$ λ would take the

value $\lambda = 10^{-3}$. We now use the fact that $C(x)$ is an odd function to

simplify (2.19) - (2.24): If we substitute

(2.28) $\qquad \overline{\psi}(x,t) = \psi(x,t) - \frac{1}{2} (\psi_1(t) + \psi_{-1}(t)) \quad .$

Equations (2.19) - (2.21) remain unchanged.

The boundary conditions (2.22) become

(2.29) $\qquad \overline{\psi}(1,t) = -\overline{\psi}(-1,t) = \frac{1}{2} (\psi_1(t) - \psi_{-1}(t)) =: \overline{\psi}_1(t)$

and the initial condition for ψ in (2.24) has to be replaced by

(2.30) $\qquad \overline{\psi}(x,0) = \overline{\psi}^I(x) := \psi^I(x) - \frac{1}{2} (\psi_1(0) + \psi_{-1}(0)) \quad .$

(2.19) - (2.23) can now be simplified by the "Ansatz"

(2.31) $\quad \bar{\psi}(-x,t) = -\bar{\psi}(x,t), \; n(-x,t) = p(x,t), \; J_n(-x,t) = J_p(x,t) \quad .$

For the rest of this paper we assume that this "Ansatz" is compatible with the

initial conditions (2.24). Thus we make the

(2.32) Assumption: ψ^I, n^I and p^I in (2.24) satisfy

(2.33) $\quad \psi^I(x) = -\psi^I(-x) + \psi^I(1) + \psi^I(-1), \; n^I(x) = p^I(-x) \quad .$

The "Ansatz" (2.31) gives the conditions

(2.34) $\quad \bar{\psi}(0,t) = 0, \; n(0,t) = p(0,t), \; J_n(0,t) = J_p(0,t) \quad .$

Thus we obtain the simplified problem on $[0,1]$

(2.35) $\lambda^2 \psi_{xx} = n - p - C$

(2.36) $n_t = J_{n_x} + R$

(2.37) $p_t = -J_{p_x} + R$

(2.38) $J_n = n_x - n\psi_x$

(2.39) $J_p = -p_x - p\psi_x$

$\qquad x \in [0,1]$

(2.40) $\psi(0,t) = 0, \; n(0,t) = p(0,t), \; J_n(0,t) = J_p(0,t)$

(2.41) $\psi(1,t) = \psi_1(t), \; n(1,t) = \frac{1}{2} (C(1) + \sqrt{C(1)^2 + 4\alpha^2}) \quad ,$

$\qquad p(1,t) = \frac{1}{2} (-C(1) + \sqrt{C(1)^2 + 4\alpha^2})$

(2.42) $\psi(x,0) = \psi^I(x) \; , \; n(x,0) = n^I(x), \; p(x,0) = p^I(x)$

(where for simplicity we have written ψ, ψ_1, ψ^I instead of $\bar{\psi}$, $\bar{\psi}_1$ and $\bar{\psi}^I$).

Remark: The reason, why (2.35) – (2.42) is simpler than (2.19) – (2.24), is

that the solution of (2.19) – (2.24) will exhibit an internal layer at $x = 0$

which can be treated as a boundary layer in (2.35) – (2.42).

3. Review of the Singular Perturbation Analysis for the Steady State Case

We now review the singular perturbation analysis carried out in Markowich and Ringhofer [1982] and Markowich et al [1983a] *for the steady state problem*

$$(3.1) \qquad \lambda^2 \psi_{xx} = n - p - C$$

$$(3.2) \qquad J_{n_x} = R \quad , \quad J_n = n_x - n\psi_x$$

$$(3.3) \qquad J_{p_x} = -R \quad , \quad J_p = -p_x - p\psi_x$$

$$(3.4) \qquad R = (np - \alpha^2)(n+p + 2\alpha)^{-1}$$

$$(3.5) \qquad \psi(0) = 0 \quad , \quad \psi(1) = \psi_1$$

$$(3.6) \qquad n = \frac{1}{2} (C + \sqrt{C^2 + 4\alpha^2}), \quad p = \frac{1}{2} (-C + \sqrt{C^2 + 4\alpha^2}), \quad x = \pm 1 \quad .$$

The purpose of this review is twofold: On one hand there will be a fair amounbt of analogy between the asymptotic behavior of (3.1) – (3.6) and the behavior of (2.35) – (2.42) on the "slow" time scale. On the other hand the initial values ψ^I, n^I and p^I in (2.42) will usually be the solutions of the steady state problem (3.1) – (3.6) and it is thus important to know their structure. Markowich and Ringhofer [1982] derived an asymptotic expansion for the problem (3.1) – (3.6) in powers of λ. This expansion is of the form

$$(3.7) \qquad w(x,\lambda) \sim \sum_{i=0}^{\infty} [\tilde{w}_i(x) + \hat{w}_i(x/\lambda)]\lambda^i$$

$$(3.8) \qquad w = (\psi,n,p,J_n,J_p)^T \quad .$$

Thus the solution of (3.1) – (3.6) can be represented as the sum of a smooth part (which has an asymptotic expansion $\sum_{i=0}^{\infty} \tilde{w}_i(x)\lambda^i$) and a boundary layer term at $x = 0$ which varies on the space scale x/λ and has an asymptotic expansion of the form $\sum_{i=0}^{\infty} \hat{w}_i(x/\lambda)\lambda^i$. The solution of the reduced problem $\tilde{w}_0$ satisfies the equations

(3.9)
$$0 = \tilde{n}_0 - \tilde{p}_0 - C$$

(3.10)
$$\tilde{J}_{n_{0_x}} = R(\tilde{n}_0, \tilde{p}_0) \quad , \quad \tilde{J}_{p_{0_x}} = -R(\tilde{n}_0, \tilde{p}_0)$$

(3.11)
$$\tilde{J}_{n_0} = \tilde{n}_{0_x} - \tilde{n}_0 \tilde{\psi}_{0_x} \quad , \quad \tilde{J}_{p_0} = -\tilde{p}_{0_x} - \tilde{p}_0 \tilde{\psi}_{0_x} \quad .$$

(3.10) - (3.11) is a system of 2 second order ordinary differential equations (obtained by inserting the expressions (3.11) for the current densities J_n and J_p into the continuity equations (3.10)) coupled to the algebraic condition (3.9). Thus we can impose two boundary conditions at each of the boundaries $x = 0$ and $x = 1$. These boundary conditions are

(3.12)
$$\exp[-\tilde{\psi}_0(0)]\tilde{n}_0(0) = \exp[\tilde{\psi}_0(0)]\tilde{p}_0(0)$$

(3.13)
$$\tilde{J}_{n_0}(0) = \tilde{J}_{p_0}(0)$$

(3.14)
$$\tilde{\psi}_0(1) = \psi_1 \quad , \quad \tilde{p}_1 = \frac{1}{2}\left(-C + \overline{\sqrt{C^2 + \psi\alpha^2}}\right) \quad .$$

Note that the boundary conditions (3.14) together with (3.9) imply the third boundary condition $n = \frac{1}{2}\left(C + \overline{\sqrt{C^2 + 4\alpha^2}}\right)$ in (2.41). This is why no boundary layer occurs at $x = 1$. The zeroth order layer term $\hat{w}_0$ satisfies the relations

(3.15) $\hat{n}_0(\zeta) = \tilde{n}_0(0)\{\exp[\hat{\psi}_0(\zeta)] - 1\}$, $\hat{p}_0(\zeta) = \tilde{p}_0(0)\{\exp[-\hat{\psi}_0(\zeta)] - 1\}$

(3.16) $\hat{J}_{n_0}(\zeta) = \hat{J}_{p_0}(\zeta) = 0$

$$\zeta := x/\Lambda \quad .$$

$\hat{\psi}_0$ satisfies the second order o.d.e. problem

(3.17) $\hat{\psi}_{0_{\zeta\zeta}} = \hat{n}_0 - \hat{p}_0 = \tilde{n}_0(0)[e^{\hat{\psi}_0} - 1] - \tilde{p}_0(0)[e^{-\hat{\psi}_0} - 1]$

(3.18) $\hat{\psi}_0(0) = -\tilde{\psi}_0(0)$, $\hat{\psi}_0(\infty) = 0 \quad .$

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Thus for the zeroth order approximation of w we have a boundary layer at $x = 0$ in the variables ψ, n and p. J_n and J_p do not exhibit a boundary layer at $x = 0$.

4. Asymptotic Analysis for the Time Dependent Problem

In this chapter we carry out our asymptotic analysis for the solution of (1.1) – (1.12) as λ tends to zero. As we will see the choice of initial conditions crucially influences the asymptotic behavior of (1.1) – (1.12). We assume that the initial values ψ^I, n^I and p^I have an asymptotic expansion of the form

$$(4.1) \qquad w^I(x,\lambda) \approx \sum_{i=0}^{\infty} [\tilde{w}_i^I(x) + \hat{w}^I(\tfrac{x}{\lambda})]\lambda^i$$

$$w^I = (\psi^I, n^I, p^I)^T, \quad |\hat{w}^I(\zeta)| < C_1 \exp(-C_2\zeta) \quad .$$

This choice is of course motivated by the structure of the solutions of the steady state problem (1.17) – (1.20). First we derive our asymptotic expansion for the solution of (1.1) – (1.12) which varies on the slow time scale t_i i.e.

$$(4.2) \qquad w(x,t,\lambda) \sim \sum_{i=0}^{\infty} [\tilde{w}_i(x,t) + \hat{w}_i(\tfrac{x}{\lambda},t)]\lambda^i \quad .$$

In order for this expansion to be valid, it will be necessary to impose certain restrictions on the initial values ψ^I, n^I and p^I. These conditions will be satisfied if $\psi_.^I$, n^I and p^I are the solutions of the steady state problem (1.17) – (1.20). The zeroth order term $\tilde{w}_0$ of the outer solution satisfies

$$(4.3) \qquad 0 = \tilde{n}_0 - \tilde{p}_0 - C$$

$$(4.4) \qquad \text{(a)} \ \tilde{n}_{0_t} = \tilde{J}_{n_{0_x}} - R(\tilde{n}_0, \tilde{p}_0), \quad \text{(b)} \ \tilde{p}_{0_t} = -\tilde{J}_{p_{0_x}} - R(\tilde{n}_0, \tilde{p}_0)$$

$$(4.5) \qquad \text{(a)} \ J_n = \tilde{n}_{0_x} - \tilde{n}_0 \tilde{\psi}_{0_x}, \quad \text{(b)} \ J_p = -\tilde{p}_{0_x} - \tilde{p}_0 \tilde{\psi}_{0_x} \quad .$$

Substracting (4.4)(b) from (4.4)(a) and replacing $\tilde{n}_0$ by $\tilde{p}_0 + C$ gives

$$(4.6) \qquad 0 = \mathfrak{J}_{0_x}, \quad \mathfrak{J}_0 = \mathfrak{J}_{n_0} + \mathfrak{J}_{p_0} = C_x - (2\tilde{p}_0 + C)\tilde{\psi}_{0_x}$$

$$(4.7) \qquad \tilde{p}_{0_t} = -\mathfrak{J}_{p_{0_x}} - R(\tilde{p}_0 + C, \tilde{p}_0), \quad \mathfrak{J}_{p_0} = -\tilde{p}_{0_x} - \tilde{p}_0\tilde{\psi}_{0_x} \quad .$$

(4.6) is now a second order elliptic equation for $\tilde{\psi}_0$ coupled to the parabolic equation (4.7) for $\tilde{p}_0$. Thus we can impose two boundary conditions at each boundary $x = 0$ and $x = 1$. At $x = 1$ we impose the conditions

$$(4.8) \qquad \tilde{\psi}_0(1,t) = \psi_1(t), \quad \tilde{p}_0(1,t) - \frac{1}{2}(C + \sqrt{C^2 + 4\alpha^2}) \quad .$$

Note that – as in the steady state case – (4.8) together with (4.3) implies the third boundary condition $\tilde{n}_0(1,t) = \frac{1}{2}(C(1) + \sqrt{C(1)^2 + 4\alpha^2})$ in (2.41). Thus we have satisfied all three boundary conditions at $x = 1$ with $\tilde{w}_0$. This is the reason why there is no boundary layer at $x = 1$. Inserting $\tilde{w}_0(x) + \hat{w}_0(\zeta)$ into equations (2.35) – (2.42) gives

$$(4.9) \qquad \hat{\psi}_{0_{\zeta\zeta}} = \hat{n}_0 - \hat{p}_0 - \lambda^2 \tilde{\psi}_{0_{xx}}$$

$$(4.10) \qquad \hat{\mathfrak{J}}_{n_{0_\zeta}} = \lambda [\hat{n}_{0_t} + R(\tilde{n}_0 + \hat{n}_0, \tilde{p}_0 + \hat{p}_0) - R(\tilde{n}_0, \tilde{p}_0)]$$

$$(4.11) \qquad \hat{\mathfrak{J}}_{p_{0_\zeta}} = \lambda [-\hat{p}_{0_t} - R(\tilde{n}_0 + \hat{n}_0, \tilde{p}_0 + \hat{p}_0) + R(\tilde{n}_0, \tilde{p}_0)]$$

$$(4.12) \qquad \lambda\hat{\mathfrak{J}}_{n_0} = \hat{n}_{0_\zeta} - (\tilde{n}_0 + \hat{n}_0)\hat{\psi}_{0_\zeta} - \lambda\hat{n}_0\tilde{\psi}_{0_x}$$

$$(4.13) \qquad \lambda\hat{\mathfrak{J}}_{p_0} = -\hat{p}_{0_\zeta} - (\tilde{p}_0 + \hat{p}_0)\hat{\psi}_{0_\zeta} - \lambda\hat{p}_0\tilde{\psi}_{0_x} \quad .$$

$\lambda \to 0$ gives

$$(4.14) \qquad \hat{\psi}_{0_{\zeta\zeta}} = \hat{n}_0 - \hat{p}_0$$

$$(4.15) \qquad \hat{\mathfrak{J}}_{n_{0_\zeta}} = \hat{\mathfrak{J}}_{p_{0_\zeta}} = 0$$

$$(4.16) \qquad \hat{n}_{0_\zeta} - [\hat{n}_0 + \tilde{n}_0(0,t)]\hat{\psi}_{0_\zeta} = 0, \quad \hat{p}_{0_\zeta} + (\tilde{p}_0(0,t) + \hat{p}_0)\hat{\psi}_{0_\zeta} = 0 \quad .$$

Since $|\hat{w}_0(\zeta,t)| < C_1(t)\exp[-C_2(t)\zeta]$ has to hold, $w(\infty,t) = 0$ holds. Thus we can integrate (4.15) and (4.16) and obtain

$$(4.17) \qquad \hat{J}_{n_0} \equiv \hat{J}_{p_0} \equiv 0$$

$$(4.18) \qquad \hat{n}_0(\zeta,t) = \tilde{n}_0(0,t)\{\exp[\hat{\psi}_0(\zeta,t)] - 1\}$$

$$(4.19) \qquad \hat{p}_0(\zeta,t) = \tilde{p}_0(0,t)\{\exp[-\hat{\psi}_0(\zeta,t)] - 1\}$$

$$(4.20) \qquad \hat{\psi}_{0_{\zeta\zeta}} = \hat{n}_0 - \hat{p}_0 \ .$$

Inserting $\tilde{w}_0 + \hat{w}_0$ in the boundary conditions gives

$$(4.21) \qquad \hat{\psi}_0(0,t) = -\tilde{\psi}_0(0,t)$$

$$(4.22) \qquad \tilde{n}_0(0,t)\exp[\hat{\psi}_0(0,t)] = \tilde{p}_0(0,t)\exp[-\hat{\psi}_0(0,t)]$$

$$(4.23) \qquad \tilde{J}_{n_0}(0,t) = \tilde{J}_{p_0}(0,t) \ .$$

Combining (4.21) and (4.22) gives

$$(4.24) \qquad \tilde{n}(0,t)\exp[-\tilde{\psi}(0,t)] = \tilde{p}(0,t)\exp[\tilde{\psi}(0,t)]$$

which together with (4.23) gives the boundary conditions for the reduced problem at $x = 0$. We now investigate the initial conditions for the reduced equations (4.3) – (4.5). Since equation (4.6) is elliptic it has to hold also at $t = 0$. This gives the condition

$$(4.25) \qquad [C_x - (2\tilde{p}_0^I + C)\tilde{\psi}_0^I]_x = 0$$

$$(4.26) \qquad \tilde{n}_0^I(0)\exp[-\tilde{\psi}_0^I(0)] = \tilde{p}_0^I(0)\exp[\tilde{\psi}_0^I(0)]$$

$$(4.27) \qquad \tilde{\psi}_0^I(1) = \psi_1(0)$$

on the zeroth order term of $\tilde{w}^I(x,\lambda)$. Also the layer equations (4.14) – (4.16) have to hold for $t = 0$ since they are time-independent. This gives the condition

$$(4.26) \qquad \hat{n}_0^I(\zeta) = \tilde{n}_0^I(0)\{\exp[+\hat{\psi}_0^I(\zeta)] - 1\}$$

$$(4.27) \qquad \hat{p}_0^I(\zeta) = \tilde{p}_0^I(0)\{\exp[-\hat{\psi}_0^I(\zeta)] - 1\}$$

on $\hat{w}_0^I$. Equation (4.14) has to be satisfied because of the compatibility condition (2.28). Using the theory outlined in the previous chapter we see that conditions (4.24) - (4.27) are satisfied if w^I is the solution of the steady-state problem (3.1) - (3.6). Thus, if conditions (4.24) - (4.27) are satisfied we have determined the zeroth order term $\tilde{w}_0^I + \hat{w}_0^I$ of the expansion (4.2). We summarize this in the

(4.28) **Theorem:**

If $w^I(x,\lambda)$ has an asymptotic expansion $w^I \sim \sum_{i=0}^{\infty} (\tilde{w}_i^I(x) + \hat{w}_i^I(\frac{x}{\lambda}))\lambda^i$, $w^I = (\psi^I, n^I, p^I)^T$ and $\tilde{w}_0^I$ and $\hat{w}_0^I$ satisfies the conditions (4.24) - (4.27) (as it is the case if w^I is the solution of the steady state problem (4.1) - (4.6)) then the zeroth order term $\tilde{w}_0^I(x,t)$ satisfies the equations

$$(4.29) \qquad 0 = \mathfrak{J}_{0_x}, \quad \mathfrak{J}_0 = \mathfrak{J}_{n_0} + \mathfrak{J}_{p_0} = c_x - (2\tilde{p}_0 + c)\tilde{\psi}_{0_x}$$

$$(4.30) \qquad \tilde{p}_{0_t} = -\mathfrak{J}_{p_{0_x}} + R(\tilde{p}_0 + c, \tilde{p}_0), \quad \mathfrak{J}_{p_0} = -\tilde{p}_{0_x} - \tilde{p}_0 \tilde{\psi}_{0_x}$$

together with the boundary conditions

$$(4.31) \qquad [\tilde{p}(0,t) + c(0)]\exp[-\tilde{\psi}_0(0,t)] = \tilde{p}_0(0,t)\exp[\tilde{\psi}_0(0,t)]$$

$$(4.32) \qquad \tilde{\mathfrak{J}}_0(0,t) = 2\tilde{\mathfrak{J}}_{p_0}(0,t)$$

$$(4.33) \qquad \tilde{\psi}_0(1,t) = \psi_1(t), \quad \tilde{p}_0(1,t) = \frac{1}{2}(-c(1) + \sqrt{c(1)^2 + \psi\alpha^2})$$

and the initial conditions

$$(4.34) \qquad \tilde{p}_0(x,0) = \tilde{p}_0^I(x) \quad .$$

The zeroth order layer term $\hat{w}_0(\zeta,t)$ satisfies the relations

$$(4.35) \qquad \hat{n}_0(\zeta,t) = \tilde{n}_0(0,t)[\exp[\hat{\psi}_0(\zeta,t)] - 1]$$

(4.36) $\hat{p}_0(\zeta,t) = \tilde{p}_0(0,t)[\exp[-\hat{\psi}_0(\zeta,t)] - 1]$

(4.37) $\hat{J}_{n_0} = \hat{J}_{p_0} = 0$

(4.38) $\hat{\psi}_{0_{\zeta\zeta}} = \hat{n}_0 - \hat{p}_0, \ \hat{\psi}_0(0,t) = -\tilde{\psi}_0(0,t), \ \hat{\psi}_0(\infty,t) = 0$.

So we have determined the zeroth order approximation to the solution of (2.35) - (2.42) in the case that the initial functions ψ^I, n^I and p^I are solutions of the steady state problem. This expansion varies in time on the timescale t. Thus the reaction time of the p - n junction (the time it takes the system to reach another steady state if we vary the bias) will be of this order of magnitude. Essential for the derivation of this asymptotic solution was the fact that (4.24) - (4.27) was satisfied for the initial values. Although this will be the case for all practical purposes (since we always start with a steady state solution) it is of some interest to see what happens if conditions (4.24) - (4.27) are violated. This is the case if we solve (2.35) - (2.42) numerically and our numerical solution is "polluted" by a discretization error. For this purpose it is convenient to rewrite our problem (2.35) - (2.42): We elliminate n from (2.36) - (2.38) by substituting $n = \lambda^2 \psi_{xx} + p + C$ in (2.36) - (2.38) and subtracting (2.37) from (2.36). This gives

(4.39) $\lambda^2 \psi_{xx} = J_x, \ J = J_n + J_p = C_x + \lambda^2 \psi_{xxx} - (2p + C + \lambda^2 \psi_{xx})\psi_x$

(4.40) $p_t = -J_{p_x} - R, \ J_p = -p_x - p\psi_x$.

We now supplement our expansion (4.2) by a term $\bar{w}(\tau,x,\lambda)$ which varies on the fast time scale $\tau = t\lambda^{-\gamma}, \ \gamma > 0$ (where γ still remains to be determined)

$$(4.41) \qquad w(x,t,\lambda) \sim \sum_{i=0}^{\infty} [\widetilde{w}_i(x,t) + \hat{w}_i(\zeta,t) + \overline{w}_i(x,\tau)]\lambda^i$$

$$(4.42) \qquad |\overline{w}_i(x,\tau)| \leqslant C_1(x)\exp(-C_2(x)\tau), \quad i = 1,2,\ldots \ .$$

Inserting (4.41) into (4.39) gives

$$\lambda^{2-\gamma}\,\overline{\psi}_{0_{xx\tau}} = [\lambda^2\,\overline{\psi}_{0_{xxx}} - (2p_0 + c + \lambda^2\psi_{0_{xx}} + 2\overline{p}_0 + \lambda^2\,\overline{\psi}_{0_{xx}})\cdot$$

(4.43)

$$\overline{\psi}_{0_x} - (2\overline{p}_0 + \lambda^2\,\overline{\psi}_{0_{xx}})\psi_{0_x}]_x$$

$$(4.44) \qquad \overline{p}_{0_\tau} = \lambda^\gamma\,\overline{J}_{p_{0_x}}, \quad \overline{J}_{p_0} = -\overline{p}_{0_x} - (p_0 + \overline{p}_0)\overline{\psi}_{0_x} - p_0\psi_{0_x}$$

where ψ_0 and p_0 stand for the zeroth order expansion on the slow timescale t.

$$(4.45) \qquad \psi_0 = \widetilde{\psi}_0)x,\lambda^\gamma\tau) + \overset{\wedge}{\psi}_0(\zeta,\lambda^\gamma\tau)$$

$$(4.46) \qquad p_0 = \widetilde{p}_0(x,\lambda^\gamma\tau) + \hat{p}_0(\zeta,\lambda^\gamma\tau) \ .$$

$\lambda \to 0$ in (4.44) gives $\overline{p}_{0_\tau} = 0$ which together with (4.42) implies $\overline{p}_0 \equiv 0$. From (4.43) we see that the only value of γ which produces a nontrivial solution away from $x = 0$ is $\gamma = 2$.

Thus we set $\tau = \dfrac{t}{\lambda^2}$ and let λ tend to zero in (4.43) - (4.44). This gives

$$(4.47) \qquad \overline{\psi}_{0_{xx\tau}} = -\big[(2p_0 + c)\overline{\psi}_{0_x}\big]_x$$

$$(4.48) \qquad \overline{p}_0 \equiv 0 \ .$$

For a complete asymptotic expansion in the case of general initial conditions we refer the reader to Ringhofer [1983].

5. Finite Difference Methods

In this chapter we develop a finite difference scheme for the solution of problem (1.1) - (1.12). Severe stability problems arise because of the presence of the fast time scale (t/λ^2) in (4.47). To illustrate this we first consider a "naive" discretization of (2.35) - (2.42): First we only discretize (2.35) - (2.42) in time and leave the space variable x continuous. Thus we define a sequence

$$(5.1) \qquad \{t_k, \ 0 = t_0 < \ldots < t_k < \ldots \ \}, \ \Delta t_k := t_{k+1} - t_k, \ k = 0,1,\ldots$$

and denote the function $v(x,t_k)$ with

$$(5.2) \qquad v^k(x) = v(t_k,x), \ v = (\psi,n,p,J_n,J_p)^T, \ k = 0,1,\ldots \ .$$

As a first approach one would perhaps try to solve equations (2.35) - (2.42) by a Crank-Nicholson scheme and solve Poisson's equation (2.35) implicitly on the new time level. This would give

$$(5.3) \qquad \lambda^2 \psi^{k+1}_{xx} = n^{k+1} - p^{k+1} - C$$

$$(5.4) \qquad \frac{n^{k+1}-n^k}{\Delta t_k} = \frac{1}{2}\left(J^{k+1}_{n_x} + J^k_{n_x}\right)$$

$$(5.5) \qquad \frac{p^{k+1}-p^k}{\Delta t_k} = -\frac{1}{2}\left(J^{k+1}_{p_x} + J^k_{p_x}\right)$$

$$(5.6) \qquad J^\ell_n = n^\ell_x - n^\ell \psi^\ell_x$$

$$\ell = k, \ k+1$$

$$(5.7) \qquad J^\ell_p = -p^\ell_x - p^\ell \psi^\ell_x \ .$$

As we saw in chapter 4 the part of the potential ψ varying on the fast time scale (t/λ^2) satisfies the equation

$$\lambda^2 \psi_{xxt} = [C_x - (n+p)\psi_x]_x \ .$$

Time differencing equation (5.3) and inserting the expressions $n^{k+1} - n^k$, $p^{k+1} - p^k$ from (5.4) - (5.7) yields

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$$(5.8)\lambda^2 \frac{\psi_{xx}^{k+1} - \psi_{xx}^k}{\Delta t_k} = \frac{1}{2}[2C_x - (n^{k+1} + p^{k+1})\psi_x^{k+1} - (n^k + p^k)\psi_x^k]_x + O(\lambda^2) \quad .$$

Thus away from the boundary layer at $x = 0$, ψ_{xx}^k will behave like the
solution y^k of

$$(5.9) \qquad \lambda^2 \frac{y^{k+1} - y^k}{\Delta t_k} = -\frac{1}{2}(a^k y^k + a^{k+1} y^{k+1}) + f^k, \quad a_k > 0$$

which oscillates wildly unless $\dfrac{\Delta t_k}{\lambda^2} <$ const holds. To derive a scheme which

does not need this severe restriction on the time steps we rewrite (2.35) –
(2.42): We proceed as follows: We first discretize (2.35) – (2.42) in the
space variable x. Thus we define a mesh X and a meshsize h by

$$(5.10) \qquad X := \{x_i : x_i = ih, \; i = 0(1)N\}, \; h = \frac{1}{N} \quad .$$

(For the sake of simplicity we assume a uniform grid. The generalization of
our results to nonuniform grids is straightforward.) Realistically we have to
assume that $h \gg \lambda$ holds.

We approximate $(\psi, n, p)^T$ at x_i by the gridfunction $\{\psi_i, n_i, p_i\}^T$,
$i = 0(1)N\}$ We approximate the currents (J_n, J_p) at $x_{i+\frac{1}{2}} := (x_i + x_{i+1})/2$

by $\{(J_{n_{i+\frac{1}{2}}}, J_{p_{i+\frac{1}{2}}}), \; i = 0(1)N-1\}$. For a gridfunction $\{z_i, \; i = 0(1)N\}$ we

define the discrete operators D_+, D_- and M by

$$(5.11) \qquad (D_+z)_i = z_{i+1} - z_i, \; (D_-z)_i = z_i - z_{i-1}$$

$$(5.12) \qquad (Mz)_i = \frac{1}{2}(z_i + z_{i+1}) \quad .$$

We discretize (1.1), (1.2) and (1.3) by

$$(5.13) \qquad \lambda^2 h^{-2}(D_+D_-\psi)_i = n_i - p_i - C(x_i)$$

$$(5.14) \qquad \frac{d}{dt} n_i = (J_{n_{i+\frac{1}{2}}} - J_{n_{i-\frac{1}{2}}})/h$$

$$(5.15) \qquad \frac{d}{dt} p_i = -\left(J_{p_{i+\frac{1}{2}}} - J_{p_{i-\frac{1}{2}}}\right)/h \quad .$$

For simplicity we set the recombination rate $R = \emptyset$. For the discretization of the current relations (2.38), (2.39) we use an exponentially fitted scheme. This scheme was first proposed by Scharfetter and Gummel [1969] and analyzed in a singular perturbation framework by Markowich et al [1983b]:

$$(5.16) \qquad J_{n_{i+\frac{1}{2}}} = [\sigma(D_+\psi_i)(D_+n_i) - (Mn_i)(D_+\psi_i)]/h_i$$

$$(5.17) \qquad J_{p_{i+\frac{1}{2}}} = [-\sigma(D_+\psi_i)(D_+p_i) - (Mp_i)(D_+\psi_i)]/h_i$$

$$\sigma(z) := \frac{z}{2} \coth(z) \quad .$$

The boundary conditions transform to

$$(5.18) \quad \psi_0(t) = 0, \ n_0(t) = p_0(t), \ J_{n_{\frac{1}{2}}}(t) = J_{p_{\frac{1}{2}}}(t)$$

$$(5.19) \quad \psi_N(t) = \psi_b(t), \ p_N(t) = \frac{1}{2}\left(-C(1) + \sqrt{C(1)^2 + 4\alpha^2}\right), \ m_N(t) = p_N(t) + C(1)$$

and as initial conditions we impose

$$(5.20) \qquad \psi_i(0) = \psi_i^0, \ n_i(0) = n_i^0, \ p_i(0) = p_i^0, \ i = 1(1)N-1 \quad .$$

Where for the sake of compatibility we assume

$$(5.21) \qquad \lambda^2 h^{-2} D_+ D_- \psi_i^0 = n_i^0 - p_i^0 - C(x_i), \ i = 2(1)N-1 \quad .$$

(5.13) - (5.20) is an initial value problem for a system of $2(N-1)$ ordinary differential equations coupled to the $N - 1$ algebraic equations (5.13). We now eliminate the algebraic equations (5.13) by differentiating (5.13) with respect to t and inserting for n_t and p_t from (5.14) and (5.15). We obtain

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$$(5.22) \qquad \lambda^2 h^{-2} D_+ D_- \frac{d}{dt} \psi_i = \left(J_{i+\frac{1}{2}} - J_{i-\frac{1}{2}} \right)/h$$

$$(5.23) \qquad J_{i+\frac{1}{2}} = J_{n_{i+\frac{1}{2}}} + J_{p_{i+\frac{1}{2}}} = [\sigma(D_+ \psi_i)(D_+ n_i - D_+ p_i) - $$

$$(M n_i + M p_i)(D_+ \psi_i)]/h \quad .$$

We now eliminate n_i from (5.23) by using (5.13) and the boundary conditions (5.18), (5.19)

$$(5.24) \qquad n_i = p_i + v_i C(x_i) + w_i \lambda^2 h^{-2} D_+ D_- \psi_i$$

$$(5.25) \qquad w_i := \begin{cases} 1 & i \neq 0, N \\ 0 & i = 0, N \end{cases}, \quad v_i = \begin{cases} 1 & i \neq 0 \\ 0 & i = \emptyset \end{cases} .$$

Thus we obtain the system

$$(5.26) \qquad \lambda^2 h^{-1} (D_+ D_- \frac{d}{dt} \psi_i)_i = \left(J_{i+\frac{1}{2}} - J_{i-\frac{1}{2}} \right)$$

$$(5.27) \qquad h J_{i+\frac{1}{2}} = \{\sigma(D_+ \psi_i) D_+ (C(x_i)) - M(2p+C)_i (D_+ \psi_i)_i + $$

$$+ \lambda^2 h^{-2} [\sigma(D_+ \psi_i) D_+ (w D_+ D_- \psi)_i - (M(w D_+ D_- \psi))_i (D_+ \psi)_i]\}$$

which approximates the fourth order differential equation

$$(5.28) \qquad \lambda^2 \psi_{xxt} = J_x$$

$$(5.29) \qquad J = C_x - (2p+c)\psi_x + \lambda^2 \psi_{xxx} - \lambda^2 \psi_{xx}\psi_x \quad .$$

The problem consisting of (5.15), (5.17), (5.26), (5.27) together with the initial conditions (5.20) for p_i and ψ_i is equivalent to the original problem (5.13) - (5.17) if we define n_i by (5.24).

Inserting (5.24) into (5.23) we obtain

$$(5.30) \qquad \lambda^2 (D_+ D_- \frac{d}{dt} \psi)_i = D_- [\sigma(D_+ \psi)(D_+ C) - M(2p+C)(D_+ \psi)]_i + O\left(\frac{\lambda^2}{h^2}\right)$$

$$(5.31) \qquad (\frac{d}{dt} p)_i = h^{-2} D_-[\sigma(D_+\psi)(D_+p) + (Mp)(D_+\psi)]_i \ .$$

To avoid the stability problems outlined at the beginning of this chapter (5.30) has to be discretized by backward differencing. (5.31) can be discretized by the trapezoidal rule (or the Crank-Nicholson scheme). The terms abreviated with $O(\lambda^2 h^{-2})$ in (5.30) can be taken at the previous time step since we assumed $\lambda h^{-1} \ll 1$. Thus we approximate ψ_i, n_i, p_i, $J_{i+\frac{1}{2}}$,

$J_{p_{i+\frac{1}{2}}}$ at $t = t_k$ by ψ_i^k, n_i^k, p_i^k, $J_{i+\frac{1}{2}}^k$, $J_{p_{i+\frac{1}{2}}}^k$ and obtain

$$(5.32) \qquad \lambda^2(h,\Delta t)^{-1}(D_+ D_-(\psi^{k+1} - \psi^k))_i = J_{i+\frac{1}{2}}^{k+1} - J_{i-\frac{1}{2}}^{k+1}$$

$$(5.33) \qquad (\Delta t)^{-1}(p_i^{k+1} - p_i^k) = \frac{1}{2}(J_{p_{i+\frac{1}{2}}}^{k+1} - J_{p_{i-\frac{1}{2}}}^{k+1} + J_{p_{i+\frac{1}{2}}}^k + J_{p_{i-\frac{1}{2}}}^k)/h$$

$$hJ_{i+\frac{1}{2}}^k = \sigma(D_+\psi_i^{k+1})(D_+C)_i - M(2p^{k+1} + C)_i(D_+\psi^{k+1})_i +$$

$$(5.34)$$

$$+ \lambda^2 h^{-2}[\sigma(D_+\psi_i^k)D_+(w(D_+D_-\psi^k))_i - M(w(D_+D_-\psi^k))_i(D_+\psi^k)_i$$

$$(5.35) \qquad hJ_{p_{i+\frac{1}{2}}}^k = -\sigma(D_+\psi_i^k)(D_+p^k)_i - (Mp^k)_i(D_+\psi^k)_i$$

$$(5.36) \qquad \psi_0^{k+1} = 0, \ \psi_N^{k+1} = \psi_b(t_{k+1})$$

$$(5.37) \qquad 2J_{p_{\frac{1}{2}}}^{k+1} = J_{\frac{1}{2}}^{k+1} \ p_N^{k+1} = p_b(t_{k+1}) = \frac{1}{2} [-C(1) + \overline{\sqrt{C(1)^2 + 4\alpha^2}}] \ .$$

This corresponds to solving the differential equations

$$(5.38) \qquad \frac{\lambda^2}{\Delta t}(\psi_{xx}^{k+1} - \psi_{xx}^k) = [C_x - (2p^{k+1} + C)\psi_x^{k+1} + \lambda^2\psi_{xxx}^k - \lambda^2\psi_{xx}^k\psi_x^k]_x$$

$$(5.39) \qquad (\Delta t)^{-1}(p^{k+1} - p^k) = \frac{1}{2}(p_x^{k+1} + p^{k+1}\psi_x^{k+1})_x - \frac{1}{2}J_{p_x}^k$$

at each time step, which represent a coupled system of two nonlinear equations for ψ and p. (5.33), (5.35) (or (5.37)) represent a second order time discretization for (5.15), (5.17) whereas (5.32), (5.34) only is a first order time discretization for (5.22), (5.23).

The time derivative in (5.22) is multiplied by λ^2. Thus the method is actually convergent of order

$$O[(\Delta t)^2 + \lambda^2 \Delta t]$$

where Δt denotes the maximal time step. Since for practical purposes $\Delta t \gg \lambda$ will hold we can say that the method is actually of second order in time. A detailed analysis of the stability and convergence properties will be the topic of a subsequent paper.

6. Numerical results

In this chapter we present numerical results for two test problems which were solved by the technique outlined in the previous chapter. The computation was performed on a VAX-780 computer in double precision (which provides 14 significant digits). The physical parameters were taken from Table 2 in Chapter 1. We took a constant doping profile on the interval $[0,\ell]$. The maximal doping ($\bar{C}$ in Chapter 2) was taken to be $10^{17} cm^{-3}$. The characteristic length 2ℓ of the device was taken to be 5μ. This corresponds to $\lambda = 10^{-3}$. As initial values the solution of the equilibrium problem (that is the steady state problem with zero bias applied) have been taken on the interval $[0,1]$. 21 equally spaced gridpoints were taken in the x direction ($h = 0.05$). As time steps we used $\Delta t_k = \Delta t = 0.1$, $k = 0,1,2,\ldots$. (No stability problems were encountered when we varied Δt.) Two cases have been simulated: First we switched from the equilibrium to a reverse bias of 0.25V. In the other case we switched from 0V. (equilibrium) to a voltage of 0.25V forward bias. This corresponds to a variation of the boundary condition $\psi_1(t)$ in (2.41) from $\psi_1 = 16.12$ ($\sim \emptyset.V$) to $\psi_1 = 21.12$ ($\sim 0.25V$ reverse bias) in figures 1, 2 and 3 an to a switch from $\psi_1 = 16.12$ ($\sim 0.V$) to $\psi_1 = 11.12$ ($\sim 0.25V$ forward bias) in figures 4, 5 and 6.

We plotted ψ and the hole density p on the interval $[0,1]$. The electron density n would be given by

$$n(x,t) = p(x,t) + C(x) + \lambda^2 \psi_{xx}(x,t) \quad .$$

Thus away from $x = 0$ it differs visually from p only by the (constant) function $C(x)$. To obtain a picture of the full solution on $[-1,1]$ ψ, n and p would have to be continued according to $\psi(-x) = -\psi(x)$, $n(-x) = p(x)$. In figures 3 and 6 we plotted the value of the total current

$$J(t) = \int_{-1}^{1} J_n(x,t) + J_p(x,t)dx$$

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as a function of time.

In detail the figures 1 - 6 show:

Figures 1 - 3: Switch from $\emptyset.V$ to $0.25V$ forward bias

Figure 1: $\psi(x,t)$, Figure 2: $\log_{10}(p(x,t))$,

Figure 3: $\log_{10}(J(t))$

Figures 4 - 6: Switch from $\emptyset.V$ to $\emptyset.25V$ forward bias
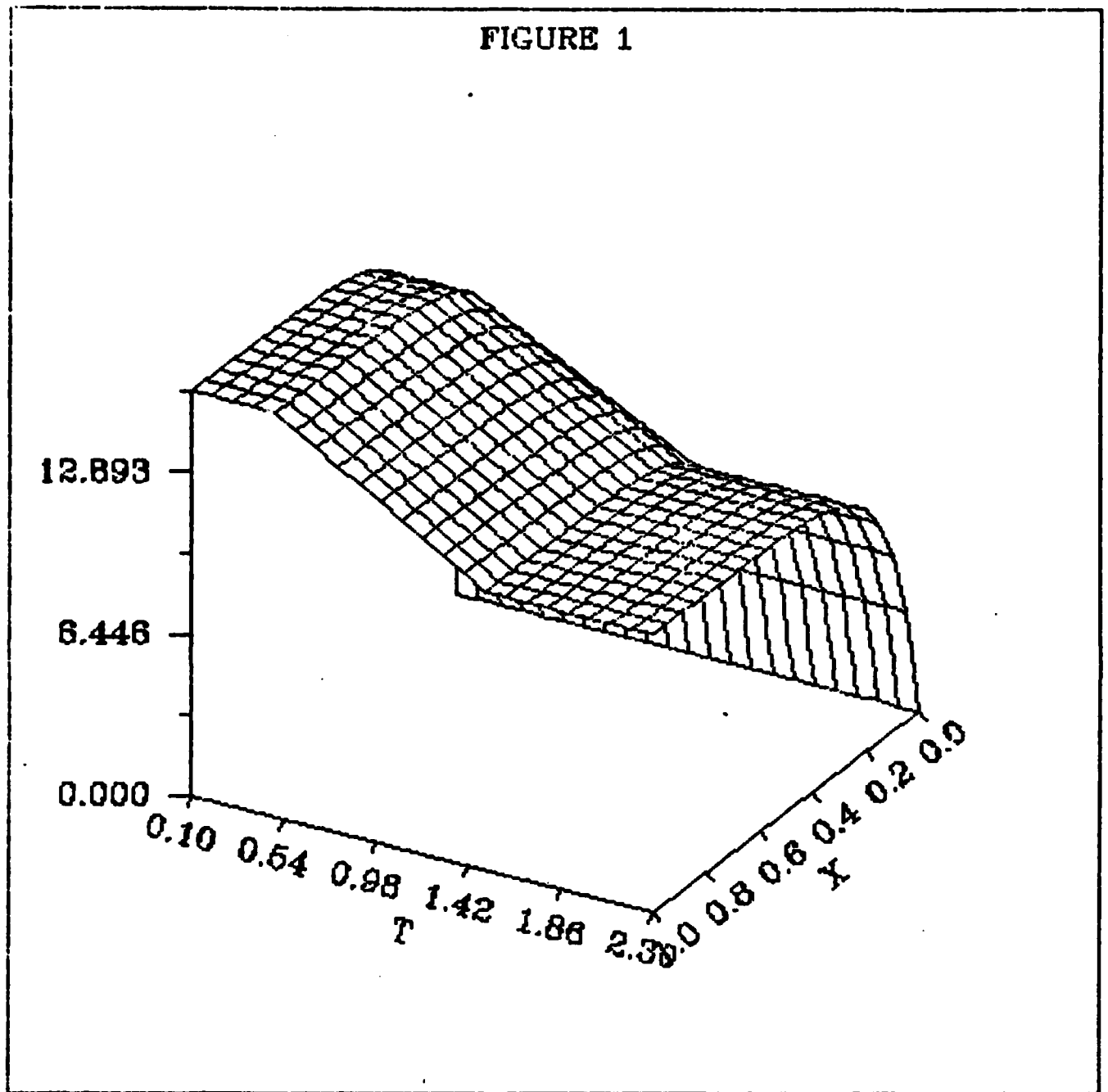
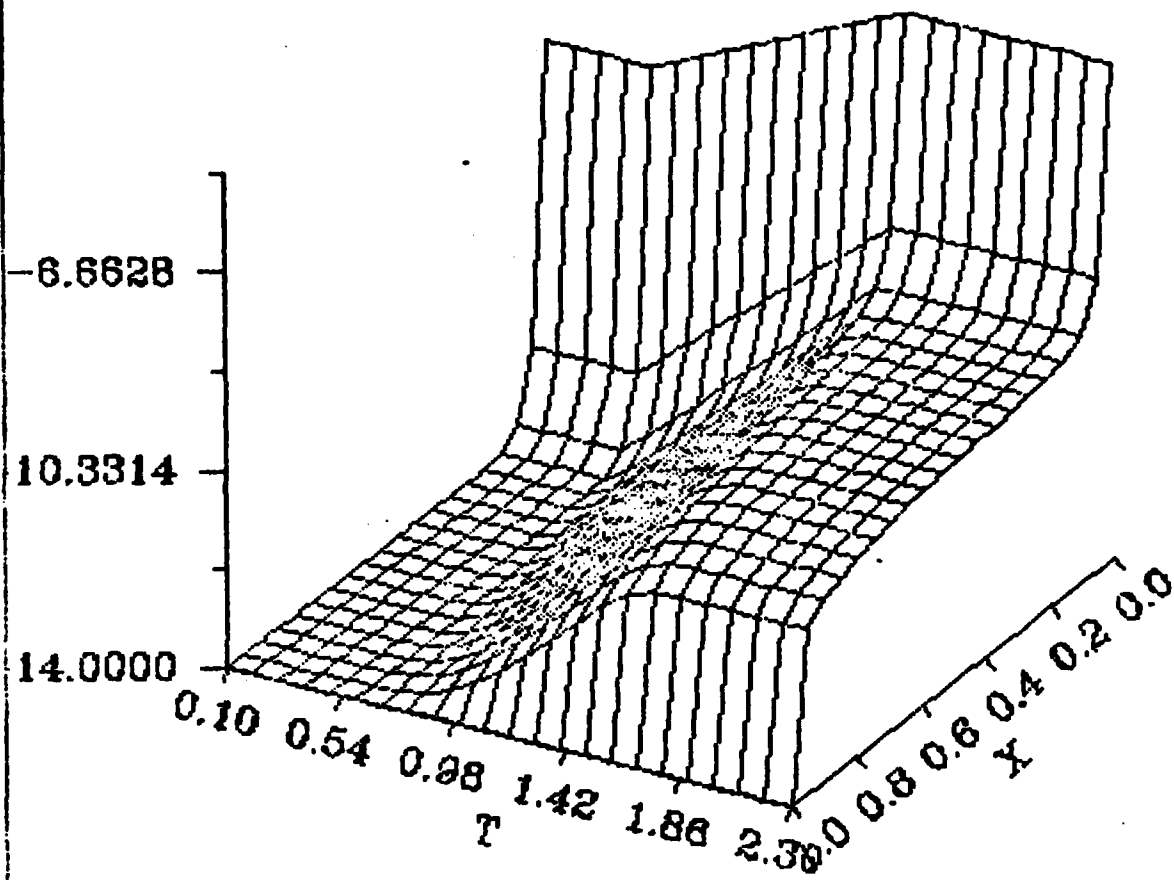Figure 4: $\psi(x,t)$, Figure 5: $\log_{10}(p(x,t)$, Figure 6: $\log_{10}(J(t))$

FIGURE 1

FIGURE 2

FIGURE 3

FIGURE 4

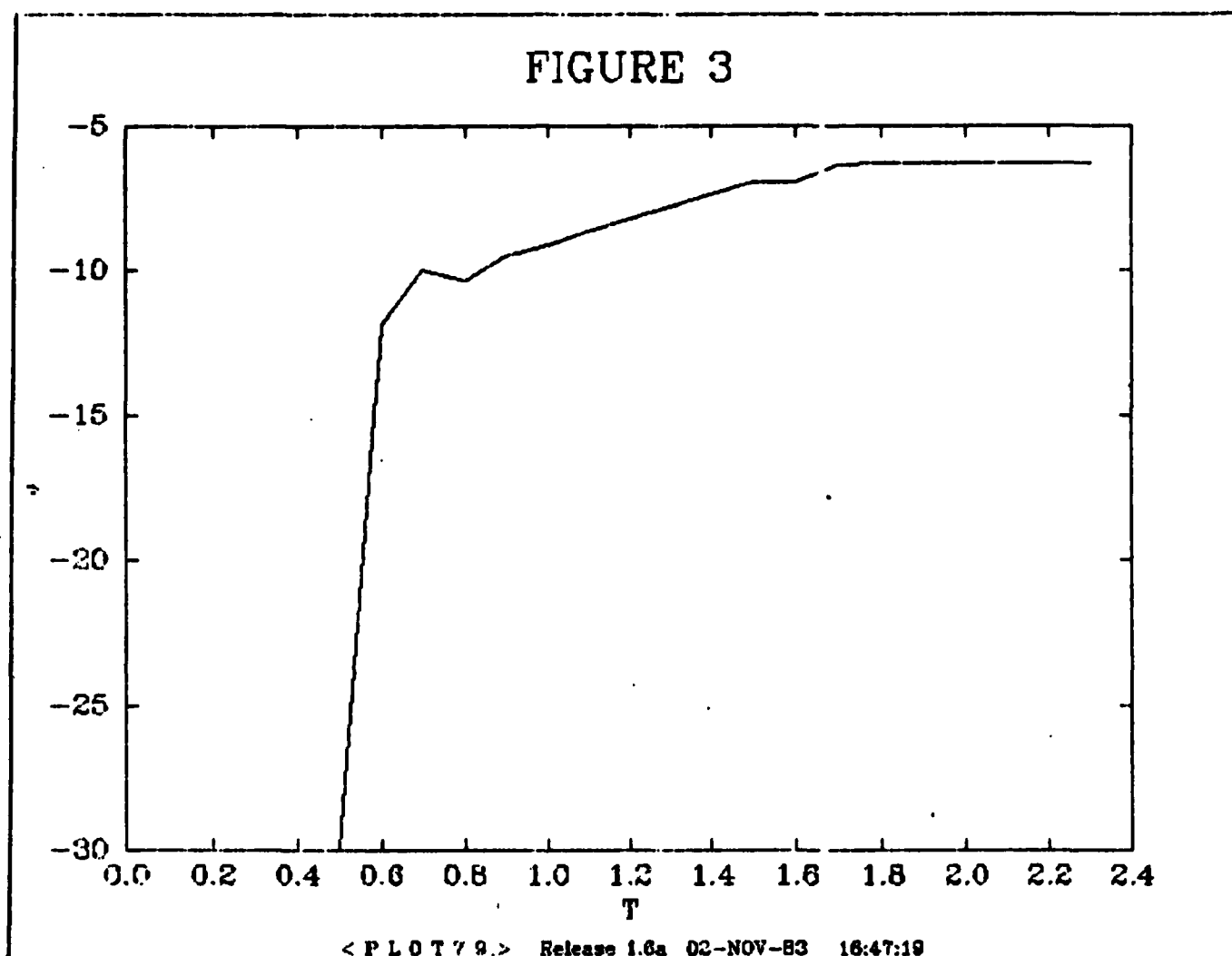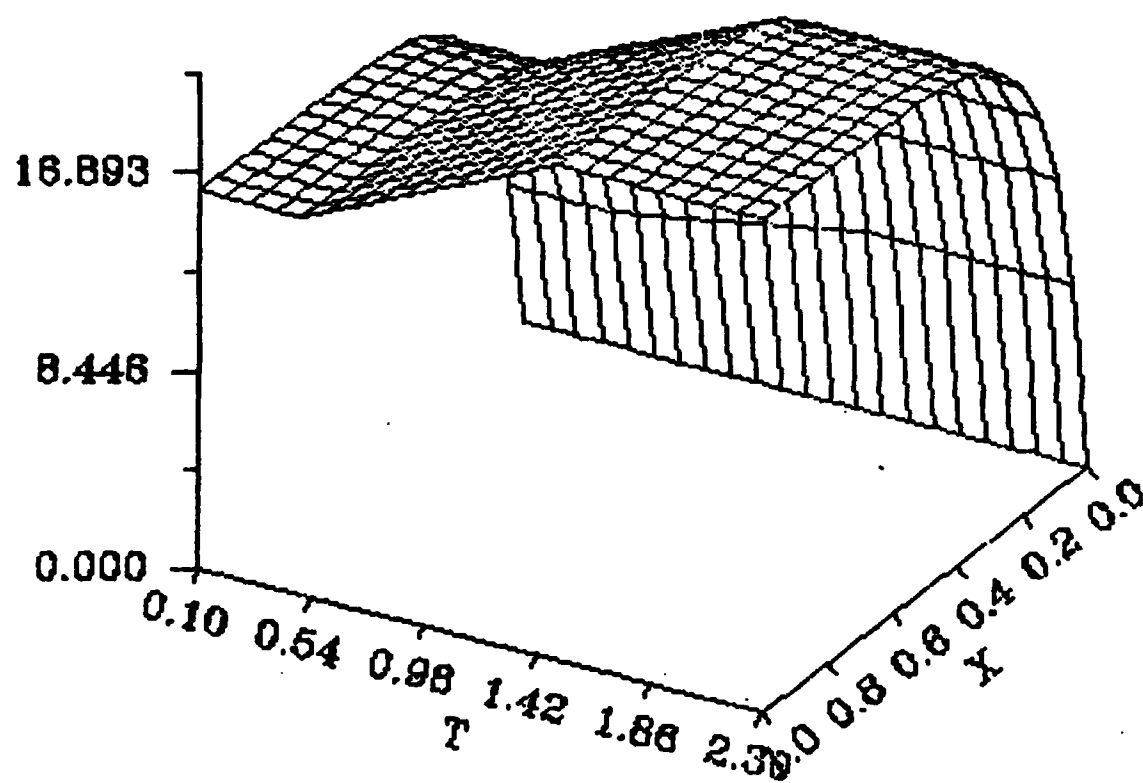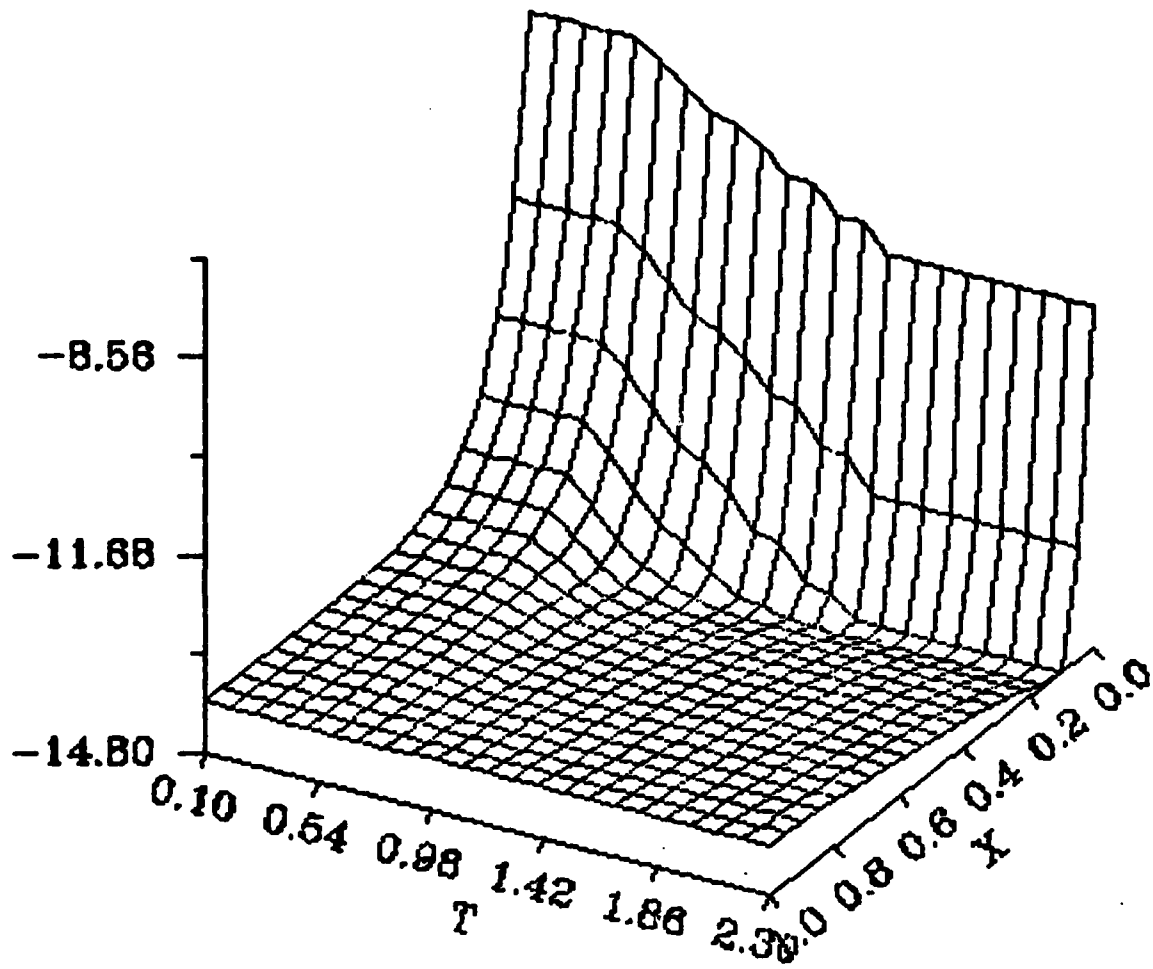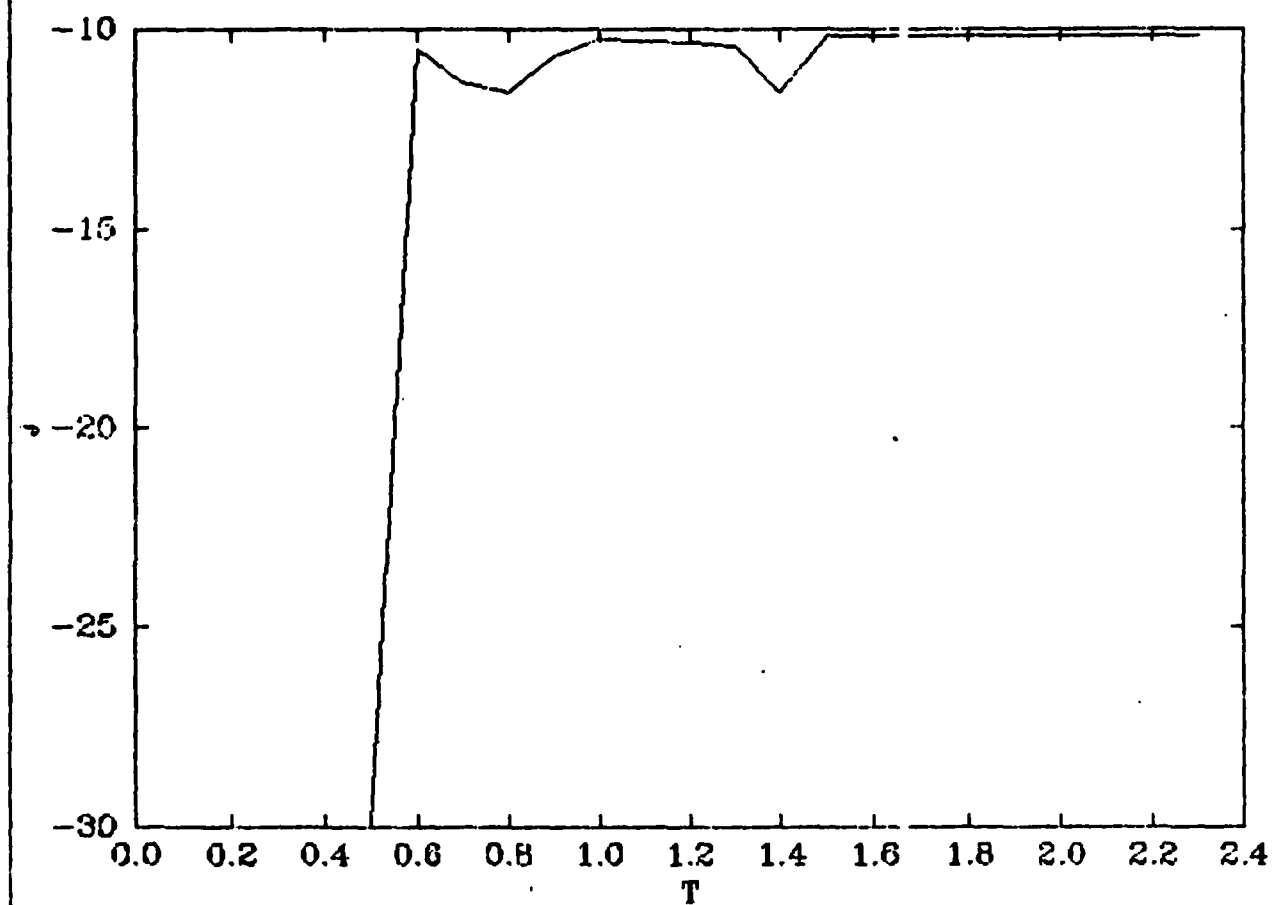FIGURE 5

FIGURE 6

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A mixed system of parabolic and elliptic partial differential equations is used to describe the carrier transport and potential distribution in semi-conductor devices such as MOSFET's, diodes e.t.c. A singular perturbation analysis of the corresponding initial boundary value problem is carried out. Asymptotic expansions of the solution in powers of the minimal Debeye length are given. Based on this analysis a finite difference method for the numerical solution of these problems is developed. Here problems arise due to different time scales which are intrinsically present in the analytical

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ABSTRACT (continued)

problem. These different time scales do not occur in the physical solutions because of special (equilibrium-) initial conditions. Nevertheless they cause severe stability problems for finite difference methods. An unconditionally stable scheme is developed which minimizes computational effort. Numerical experiments on a test problem in one space dimension are presented.

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